

Natural Cinnamic Acid Derivatives: A Comprehensive Study on Structural, Anti/Pro-Oxidant, and Environmental Impacts

Kamila Gryko ¹, Monika Kalinowska ^{1,*}, Piotr Ofman ², Renata Choińska ³, Grzegorz Świdorski ¹, Renata Świsłocka ¹ and Włodzimierz Lewandowski ¹

¹ Department of Chemistry, Biology and Biotechnology, Faculty of Civil Engineering and Environmental Sciences, Białystok University of Technology, Wiejska 45E, 15-351 Białystok, Poland;

k.gryko@pb.edu.pl (K.G.); g.swiderski@pb.edu.pl (G.Ś.); r.swislocka@pb.edu.pl (R.Ś.); w-lewando@wp.pl (W.L.)

² Department of Environmental Engineering Technology, Faculty of Civil Engineering and Environmental Sciences, Białystok University of Technology, Wiejska 45E, 15-351 Białystok, Poland; p.ofman@pb.edu.pl

³ Prof. Waław Dąbrowski Institute of Agricultural and Food Biotechnology – State Research Institute, Rakowiecka 36, 02-532 Warsaw, Poland; renata.choinska@ibprs.pl

* Correspondence: m.kalinowska@pb.edu.pl

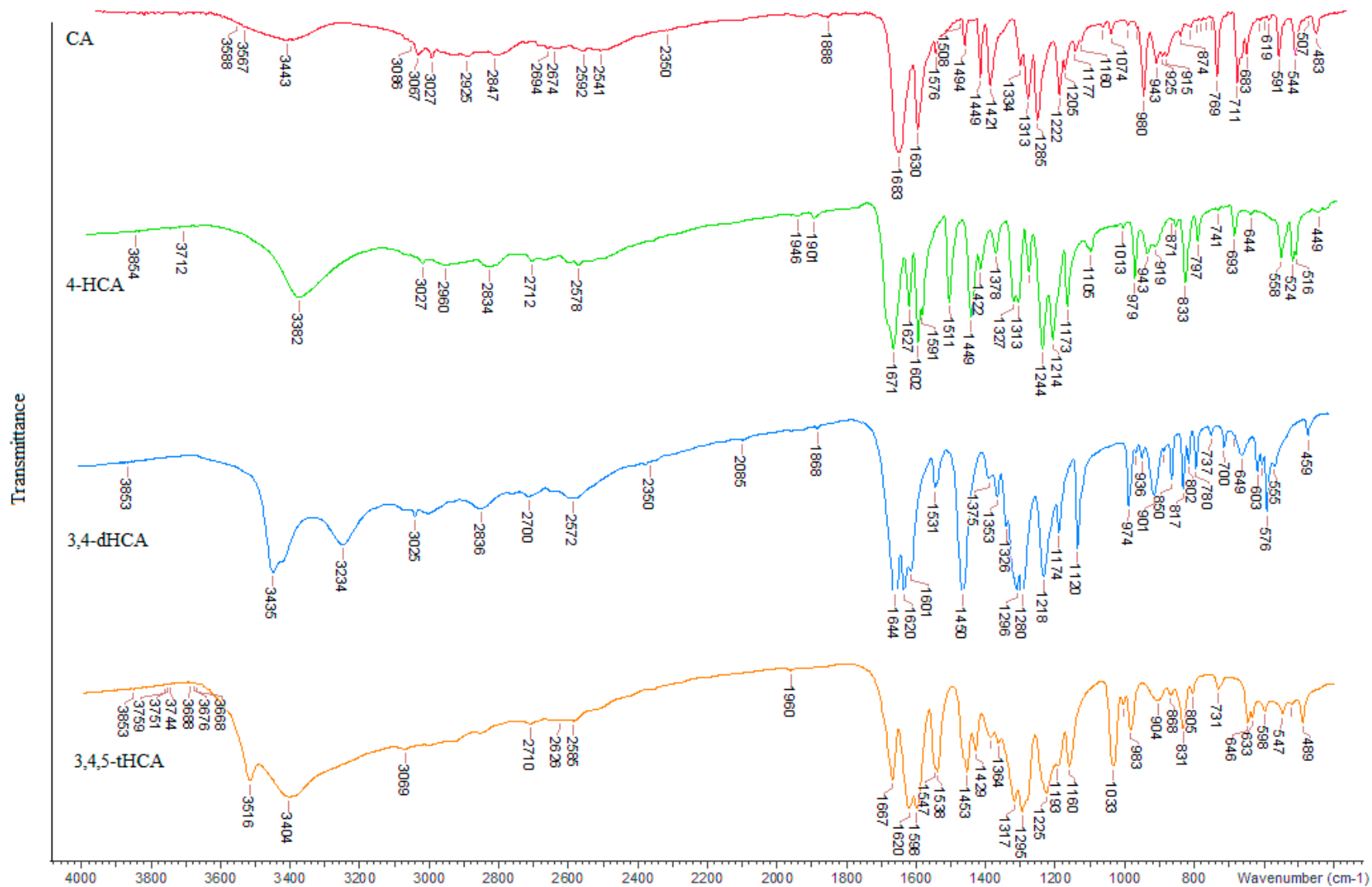


Figure S1. FT-IR spectra of CA, 4-HCA, 3,4-dHCA and 3,4,5-tHCA.

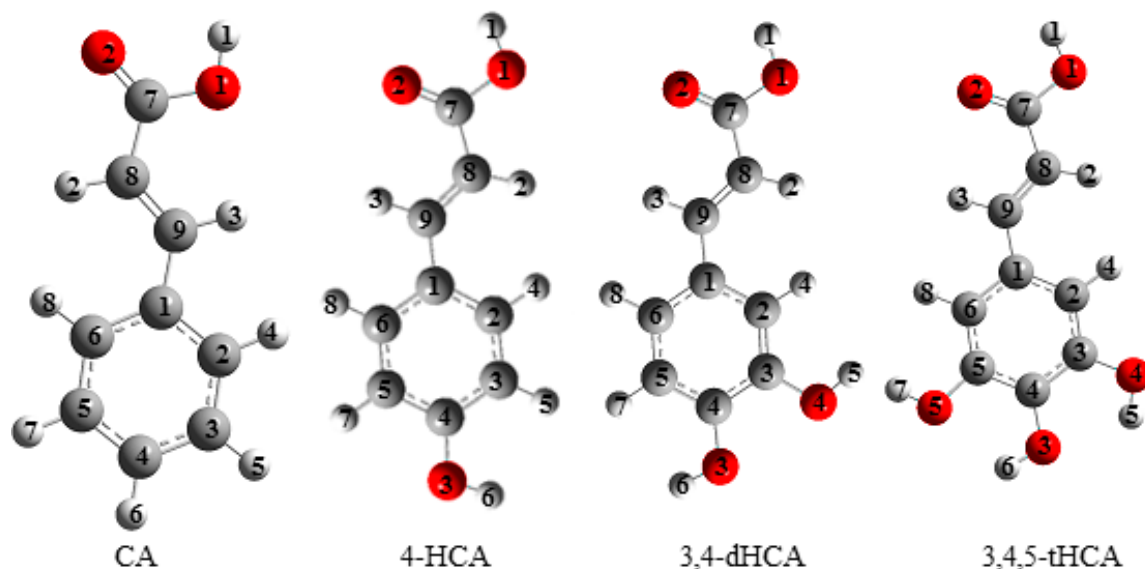


Figure S2. Atom numbering of cinnamic acid and its derivatives (structures optimized in B3LYP/6-311** (d,p) level).

Table S1. Geometrical parameters for CA, 4-HCA, 3,4-dHCA and 3,4,5-tHCA calculated in B3LYP/6-311** (d,p). Atoms numbering in Figure S2.

	CA	4-hCA	3,4-dHCA	3,4,5-tHCA
<i>Distances</i>				
C1-C2	1.40462	1.40583	1.40895	1.40383
C2-C3	1.39178	1.38618	1.38447	1.38721
C3-C4	1.39287	1.40005	1.41139	1.40005
C4-C5	1.39714	1.39552	1.39115	1.39312
C5-C6	1.38831	1.38673	1.39163	1.38794
C6-C1	1.40637	1.40683	1.40057	1.40649
C1-C9	1.46355	1.45731	1.45640	1.45889
C7-C8	1.46891	1.46948	1.46932	1.47036
C8-C9	1.34408	1.34505	1.34519	1.34418
C3-O4	-	-	1.36339	1.36054
C4-O3	-	1.36326	1.35917	1.36641
C5-O5	-	-	-	1.37578
C7-O1	1.36239	1.36333	1.36333	1.36211
C7-O2	1.21160	1.21162	1.21163	1.21183
O1-H1	0.96791	0.96840	0.96843	0.96843
O3-H6	-	0.96326	0.96331	0.96610
O4-H5	-	-	0.96304	0.96621
O5-H7	-	-	-	0.96237
C2-H4	1.08495	1.08338	1.08540	1.08191
C3-H5	1.08403	1.08585	-	-
C4-H6	1.08404	-	-	-
C5-H7	1.08411	1.08299	1.08589	-
C6-H8	1.08338	1.08474	1.08372	1.08523

Table S3. Summary of the results concerning the biological activity of the tested compounds.

Compound	DPPH• inhibition - IC ₅₀ [mM]	HO• inhibition (C=0.1mM) [%]	FRAP (C=0.05mM) [μM _{Fe2+}]	CUPRAC (C=0.05mM) [μM _{troloxu}]	Trolox pro- oxidation - 60 min (C=2.5; 5μM) [%]	Linoleic acid peroxidation inhibition - day 5. (C=5mM) [%]	E _{HOMO} [eV]	ΔE [eV]	Ionization potential [eV]
CA	> 6.0	48.40 ± 0.83	-	-	0.20 ± 1.09; 4.35 ± 0.91	30.76 ± 1.22	-9.79556	3.427	9.79556
4-HCA	> 2.7	49.99 ± 0.58	0.74 ± 0.06	6.40 ± 0.55	27.63 ± 1.58; 70.57 ± 1.18	49.49 ± 2.18	-9.18928	3.063	9.18928
3,4-dHCA	0.011 ± 0.001	50.22 ± 0.55	15.45 ± 0.49	17.99 ± 0.94	134.78 ± 4.65; 230.28 ± 1.73	82.77 ± 0.12	-8.84833	2.729	8.84833
3,4,5-tHCA	0.004 ± 0.002	53.02 ± 0.80	29.56 ± 2.02	20.86 ± 0.81	17.15 ± 0.96; 30.18 ± 0.48	88.01 ± 0.88	-8.68016	2.569	8.68016